CLAIMS

We claim:

1. A method for presenting analysis of a plurality of individual quantitative metabolite profiles, comprising:

designating the plurality of individual quantitative metabolite profiles;

identifying at least one difference or at least one similarity in a metabolite in the plurality of individual quantitative metabolite profiles; and

displaying at least one difference or at least one similarity in the metabolite in the plurality of individual quantitative metabolite profiles.

2 The method of claim 1, wherein the individual quantitative metabolite profiles are individual quantitative lipid metabolite profiles, and the method comprises:

designating the plurality of individual quantitative lipid metabolite profiles;

identifying at least one difference or at least one similarity in a lipid metabolite in the plurality of individual quantitative lipid metabolite profiles; and

displaying at least one difference or at least one similarity in the lipid metabolite in the plurality of individual quantitative lipid metabolite profiles.

3. The method of claim 2, wherein each quantitative lipid metabolite profile comprises quantitative measurements of at least two lipids and wherein the quantified measurements are obtained using an internal standard for at least one of the lipids.

4. The method of claim 3, wherein the lipid metabolites are selected from the group consisting of tetradecanoic acid, pentadecanoic acid, hexadecanoic acid, heptadecanoic acid, octadecanoic acid, eicosanoic acid, docosanoic acid, tetracosanoic acid, 9-tetradecenoic acid, 9-hexadecenoic acid, 11-octadecenoic acid, 9-octadecenoic acid, 11-eicosenoic acid, 5,8,11-eicosatrienoic acid, 13-docosenoic acid, 15-tetracosenoic acid, 9,12,15-octadecatrienoic acid, 6,9,12,15-octadecatetraenoic acid, 11,14,17-eicosatrienoic acid, 8,11,14,17-eicosictetraenoic acid, 5,8,11,14,17-eicosapentaenoic acid, 7,10,13,16,19-docosapentaenoic acid, 4,7,10,13,16,19-docosahexaenoic acid, 6,9,12,15,18,21-tetracoshexaenoic acid, 9,12-octadecadienoic acid, 6,9,12-octadecatrienoic acid, 11,14-eicosadienoic acid, 8,11,14-eicosatrienoic acid, 5,8,11,14-eicosicatetraenoic acid, 13,16-docsadienoic acid, 7,10,13,16-docosicatetraenoic acid, 4,7,10,13,16-docosapentaenoic acid, 9-trans-hexadecenoic acid, 9-trans-octadecenoic acid, 8-eicosaenoic acid, 5-eicosaenoic acid, plasmalogen fatty acids, 5b-cholestan-3b-ol, 5a-cholestan-3b-ol, 5-cholesten-3b-ol, 5,24-cholestadien-3b-ol, 5-cholestan-25a-methyl-3b-ol, 5-cholestan-24b-methyl-3b-ol, 5-cholesten-24b-ethyl-3b-ol, and 5,22-cholestadien-24b-ethyl-3b-ol, each as a compound or a component of a lipid molecule.

5. The method of claim 2, wherein the quantitative lipid metabolite profiles each comprise a quantified measurement of a lipid in a lipid class.

6. The method of claim 5, wherein the quantified measurement of the lipid in the lipid class is obtained using an internal standard for the lipid class.

7. The method of claim 5, wherein the lipid is selected from the group consisting of fatty acid 16:0, 18:0, 16:1n7; 18:1n7; 18:1n9; 18:3n3; 20:5n3; 22:5n3; 22:6n3; 18:2n6; 18:3n6; 20:3n6; and 20:4n6.

8. The method of claim 5, wherein the lipid is a sterol selected from the group consisting of 5b-cholestan-3b-ol, 5a-cholestan-3b-ol, 5-cholesten-3b-ol, 5,24-cholestadien-3b-ol, 5-cholestan-25a-methyl-3b-ol, 5-cholestan-24b-methyl-3b-ol, 5-cholesten-24b-ethyl-3b-ol, and 5,22-cholestadien-24b-ethyl-3b-ol.

9. The method of claim 5, wherein the lipid class is selected from the group consisting of lyso-phosphatidylcholine, sphingomyelin, phosphatidylcholine, phosphatidylserine, phosphatidylinositol, phosphatidylethanolamine, cardiolipin, free fatty acids, monoacylglycerides, diacylglycerides, triacylglycerides, and cholesterol esters.

10. The method of claim 6, wherein the internal standard is selected from the group consisting of diheptadecanoyl phosphatidylcholine, dipentadecaenoyl phosphatidylethanolamine, tetraheptadecenoyl cardiolipin, diheptadecenoyl phosphatidylserine, pentadecenoyl sphingomyelin, heptadecanoyl lyso-phosphatidylcholine, tripheptadecaenoyl glyceride, pentadecaenoic acid, heptadecanoic cholesterol ester and free fucosterol.

11. The method of claim 6, wherein the internal standard is heptadecanoic 1-heptadecanoyl-2-lyso-phosphatidycholine for the lipid class of lysophospholipids, N-pentadecenoyl-D-erythro-sphingosylphorylcholine for the lipid class of sphingomyelin, 1,2 diheptadecanoylphosphatidylcholine for the lipid class of phosphatidylcholine, 1,2-diheptadecenoylphosphatidylethanolamine for the lipid class of phosphatidylethanolamine, 1,2-diheptadecenoylphosphatidylserine for the lipid class of phosphatidylserine, pentadecaenoic acid for the lipid class of free fatty acids, triheptadecaenoic acid for the lipid class of triacylglycerides, 1,1',2,2'-tetraheptadecaenoyl cardiolipin for the lipid class of cardiolipin, cholesteryl heptadecanoate for the lipid class of cholesterol esters and stigmasterol for the lipid class of free sterols.

12. The method of claim 2, wherein at least one of the individual quantitative lipid metabolite profiles is generated using a method comprising:

separating a biological sample into fractions based on a plurality of lipid classes, wherein at least one quantitative internal standard is included for each lipid class; and

measuring the quantity of a plurality of lipid metabolites in the fractions.

13. The method of claim 12, wherein the plurality of lipid classes comprises lyso-phosphatidylcholines, sphingomyelins, phosphatidylcholines, phosphatidylserines, phosphatidylinositols, phosphatidylethanolamines, cardiolipins, free fatty acids, monoacylglycerides, diacylglycerides, triacylglycerides, or cholesterol esters.

14. The method of claim 12, wherein the plurality of lipid metabolites comprises at least one of tetradecanoic acid, pentadecanoic acid, hexadecanoic acid, heptadecanoic acid, octadecanoic acid, eicosanoic acid, docosanoic acid, tetracosanoic acid, 9-tetradecenoic acid, 9-hexadecenoic acid, 11-octadecenoic acid, 9-octadecenoic acid, 11-eicosenoic acid, 5,8,11-eicosatrienoic acid, 13-docosenoic acid, 15-tetracosenoic acid, 9,12,15-octadecatrienoic acid, 6,9,12,15-octadecatetraenoic acid, 11,14,17-eicosatrienoic acid, 8,11,14,17-eicosictetraenoic acid, 5,8,11,14,17-eicosapentaenoic acid, 7,10,13,16,19-docosapentaenoic acid, 4,7,10,13,16,19-docosahexaenoic acid, 6,9,12,15,18,21-tetracoshexaenoic acid, 9,12-octadecadienoic acid, 6,9,12-octadecatrienoic acid, 11,14-eicosadienoic acid, 8,11,14-eicosatrienoic acid, 5,8,11,14-eicosicatetraenoic acid, 13,16-docsadienoic acid, 7,10,13,16-docosicatetraenoic acid, 4,7,10,13,16-docosapentaenoic acid, 9-trans-hexadecenoic acid, 9-trans-octadecenoic acid, 8-eicosaenoic acid, 5-eicosaenoic acid, plasmalogen fatty acids, 5b-cholestan-3b-ol, 5a-cholestan-3b-ol, 5-cholesten-3b-ol, 5,24-cholestadien-3b-ol, 5-cholestan-25a-methyl-3b-ol, 5-cholestan-24b-methyl-3b-ol, 5-cholesten-24b-ethyl-3b-ol, or 5,22-cholestadien-24b-ethyl-3b-ol, each as a compound or a component of a lipid molecule.

15. The method of claim 12, wherein separating comprises chromatography.

16. The method of claim 12, wherein measuring comprises chromatography.

17. The method of claim 2, wherein displaying generates a web page for viewing.

18. The method of claim 17, wherein the web page comprises a representation of a heat map.

19. The method of claim 17, wherein the web page comprises a representation of a targeting chart.

20. A method of determining a metabolic effect of a condition, comprising

subjecting a subject to the condition;

taking a biological sample from the subject;

analyzing the biological sample to produce a test lipomic profile for the subject;

comparing the test lipomic profile for the subject with a control lipomic profile; and

drawing conclusions about the metabolic effect of the condition based on differences or similarities between the test lipomic profile and the control lipomic profile.

21. The method of claim 20, wherein the condition is a genotype.

22. The method of claim 21, wherein the genotype comprises a genetic knockout.

23. The method of claim 20, wherein the condition comprises a dietary limitation or supplementation.

24. The method of claim 20, wherein the condition comprises a disease or disease state.

25. The method of claim 20, wherein the condition comprises application of a toxin or suspected toxin.

26. The method of claim 20, wherein the condition comprises application of a pharmaceutical agent or candidate agent.

27. The method of claim 20, wherein the control lipomic profile is a compiled lipomic profile assembled from a plurality of individual lipomic profiles.

28. The method of claim 20, wherein the control lipomic profile is a pre-condition lipomic profile from the subject.

29. The method of claim 20, which method is a method of determining drug or treatment effectiveness, comprising

applying a drug or treatment to a subject;

taking a biological sample from the subject;

analyzing the biological sample to produce a test lipomic profile for the subject;

comparing the test lipomic profile for the subject with a control lipomic profile; and

drawing conclusions about the effectiveness of the drug or treatment based on differences or similarities between the test lipomic profile and the control lipomic profile.

30. The method of claim 29, wherein the drug or treatment is a hormone or hormone treatment.

31. The method of claim 29, wherein the drug or treatment influences obesity or diabetes.

32. The method of claim 20, which method is a method of determining likelihood of success of a treatment or procedure, comprising

subjecting a subject to the treatment or procedure;

taking a biological sample from the subject;

analyzing the biological sample to produce a test lipomic profile for the subject;

comparing the test lipomic profile for the subject with a control lipomic profile; and

drawing conclusions about the likelihood of success of a treatment or procedure based on differences or similarities between the test lipomic profile and the control lipomic profile.

33. The method of claim 32 wherein the treatment or procedure comprises an organ transplant.

34. The method of claim 32, wherein the treatment or procedure comprises a dietary limitation or supplementation.

35. The method of claim 32, wherein the treatment or procedure comprises application of a pharmaceutical agent or candidate agent.

36. A method for providing metabolic information comprising providing electronic access to the database of claim 20.

37. The method of claim 36, wherein the electronic access comprises access through the internet.

38. A method of determining the metabolic effect of an agent comprising

obtaining a quantified metabolic profile from a biological sample treated with or without an agent, wherein the quantified metabolic profile comprises a quantified measurement of a metabolite and wherein an increase or decrease of a quantified measurement of a metabolite caused by the agent is indicative of a metabolic effect of the agent.

39. The method of claim 38, wherein the agent is a therapeutic agent or a candidate therapeutic agent.

40. A method of generating a disease condition-linked quantified metabolic profile comprising

obtaining a first quantified metabolic profile from a first biological sample from a first individual having a disease condition and a second quantified metabolic profile from a second biological sample from a second individual of a normal condition, and

comparing the first quantified metabolic profile with the second quantified metabolic profile, wherein a disease condition-linked quantified metabolic profile comprises a variation of a quantified measurement of a metabolite between the first and second quantified metabolic profiles.

41. A method of diagnosing a disease condition or predisposition thereto of a subject comprising

generating a disease condition-linked quantified metabolic profile according to the method of claim 40, and

obtaining a subject quantified metabolic profile from a biological sample of a subject, wherein a subject quantified metabolic profile identical or substantially similar to the disease condition-linked quantified metabolic profile is indicative of the disease condition or the predisposition thereto.

42. A method of using a quantitative lipomic database in disease diagnosis, prognosis, or prediction, comprising screening the quantitative lipomic database for a lipid metabolite profile that is linked to the disease.

43. The method of claim 42, wherein the quantitative lipomic database is generated using a method comprising:

obtaining a plurality of quantitative lipid metabolite profiles from a plurality of biological samples, wherein each quantitative lipid metabolite profile comprises a quantified measurement of a lipid

and wherein the quantified measurement is obtained using an internal standard for the lipid so that the quantified measurement is integratable to a database, and

assembling the plurality of lipid metabolite profiles into a database.

44. A method of screening for a compound useful in treating, reducing, or preventing a disease or progression of a disease, comprising:

determining if application of a test compound alters a disease-related lipid metabolite profile so that the profile less closely resembles a disease-linked profile than it did prior to such treatment; and

selecting a compound that so alters the disease-related lipid metabolite profile,

wherein the disease-related lipid metabolite profile includes a level of at least one of the following metabolites: tetradecanoic acid, pentadecanoic acid, hexadecanoic acid, heptadecanoic acid, octadecanoic acid, eicosanoic acid, docosanoic acid, tetracosanoic acid, 9-tetradecenoic acid, 9-hexadecenoic acid, 11-octadecenoic acid, 9-octadecenoic acid, 11-eicosenoic acid, 5,8,11-eicosatrienoic acid, 13-docosenoic acid, 15-tetracosenoic acid, 9,12,15-octadecatrienoic acid, 6,9,12,15-octadecatetraenoic acid, 11,14,17-eicosatrienoic acid, 8,11,14,17-eicosictetraenoic acid, 5,8,11,14,17-eicosapentaenoic acid, 7,10,13,16,19-docosapentaenoic acid, 4,7,10,13,16,19-docosahexaenoic acid, 6,9,12,15,18,21-tetracoshexaenoic acid, 9,12-octadecadienoic acid, 6,9,12-octadecatrienoic acid, 11,14-eicosadienoic acid, 8,11,14-eicosatrienoic acid, 5,8,11,14-eicosicatetraenoic acid, 13,16-docsadienoic acid, 7,10,13,16-docosicatetraenoic acid, 4,7,10,13,16-docosapentaenoic acid, 9-tráns-hexadecenoic acid, 9-trans-octadecenoic acid, 8-eicosaenoic acid, 5-eicosaenoic acid, plasmalogen fatty acids, 5b-cholestan-3b-ol, 5a-cholestan-3b-ol, 5-cholesten-3b-ol, 5,24-cholestadien-3b-ol, 5-cholestan-25a-methyl-3b-ol, 5-cholestan-24b-methyl-3b-ol, 5-cholesten-24b-ethyl-3b-ol, or 5,22-cholestadien-24b-ethyl-3b-ol, each as a free compound or a component of a lipid molecule.

45. A method for screening for an agent having an effect on a disease condition, comprising:

obtaining a first quantified metabolic profile from a first biological sample from an individual having a disease condition and treated with a test agent, and

comparing the first quantified metabolic profile with a disease condition-linked quantified metabolic profile generated according to the method of claim 60, wherein a change in the first quantified metabolic profile caused by the test agent and associated with the disease condition-linked quantified metabolic profile is indicative that the test agent has an effect on the disease condition.

46. The method of claim 45, wherein the disease condition comprises a genotype, a dietary limitation or supplementation, a disease or disease state, a treatment with a compound, or a combination of two or more thereof.

47. A method of identifying a therapeutic target for a disease condition comprising

generating a disease condition-linked quantified metabolic profile according to the method of claim 40, wherein a variation of a quantified measurement of a metabolite is indicative of the metabolite as a therapeutic target for the disease condition.

48. The method of any one of claims 1 through 47, further comprising generating a printed report.

49. A database generated according to a method comprising:

obtaining a plurality of quantified metabolic profile from a plurality of biological samples, wherein each quantified metabolic profile comprises a quantified measurement of a metabolite and wherein the quantified measurement is obtained using an internal standard for the metabolite so that the quantified measurement is integratable to a database, and

assembling the plurality of metabolite profiles into a database,

the database comprising:

(1) a profile table including a quantified metabolic profile from a biological sample from an individual having a condition, wherein the quantified metabolic profile comprises a quantified measurement of a metabolite and wherein the quantified measurement is obtained using an internal standard for the metabolite so that the quantified measurement is integratable into a database;

(2) a sample item table including a sample record for the quantified metabolic profile;

(3) a condition item table including a condition record for the quantified metabolic profile; and

(4) a filter item table including a filter of quantified metabolic profile for a desired condition.

50. A user interface for operatively working with a processor to affect operation of the database of claim 49 comprising:

means for providing settings for selecting a set of samples,

means for providing settings for selecting a set of conditions,

means for providing settings for selecting a set of metabolites, and

means for displaying quantified metabolic profiles corresponding to the selected samples and conditions, wherein each displayed quantified metabolic profile consists of the quantified measurements of the selected metabolites.

51. The user interface of claim 50 further comprising a display area which displays the value of a quantified measurement of a metabolite within the quantified metabolic profiles of the selected samples and conditions.

52 The user interface of claim 50 further comprising

means for comparing quantified metabolic profiles corresponding to a first set of selected samples and conditions to the quantified metabolic profiles corresponding to a second set of selected samples and conditions, and

means for displaying the comparison.

53. The user interface of claim 50, the user interface comprising:

for a plurality of metabolites, a presentation of an observed quantity of at least one metabolite for a first biological sample with respect to an observed quantity of the at least one metabolite for a second biological sample, wherein the presentation is operable to accept a user indication that further information is desired with respect to a selected metabolite.